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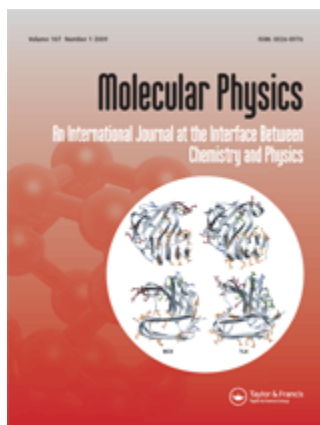
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**Torsional excitation in the 2CH vibrational overtone of the
 $C_2H_2-CO_2$ and $C_2H_2-N_2O$ van der Waals complexes**

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Abstract

Infrared spectra of the weakly-bound $C_2H_2-CO_2$ and $C_2H_2-N_2O$ complexes in the region of the 2CH acetylene overtone band ($\sim 1.52 \mu m$) were recorded using CW-cavity ring down spectroscopy in a continuous supersonic expansion. A new, *c*-type combination band is observed in each case. The rotational analysis of low *J*, *K* lines is performed and rotational constants are obtained. The band origins are $40.491(2)$ and $40.778(2) \text{ cm}^{-1}$ higher in energy than the 2CH excitation bands for $C_2H_2-CO_2$ and $C_2H_2-N_2O$, respectively. The combination band is assigned in each case as involving intermolecular torsional excitation combined to 2CH. The values of the torsional vibrational frequency and of the $x_{CH/torsion}$ anharmonicity constant are briefly discussed.

Keywords: overtone excitation, CW-CRDS, van der Waals complexes, torsion, supersonic jet, acetylene.

1. Introduction

The $C_2H_2-CO_2$ weakly bound species is known to have the two monomer units forming a planar parallel structure with C_{2v} symmetry, as presented in Figure 1. The distance between the centers of mass of the two monomers was determined to be 3.289(1) Å (1). In the nineties, this hetero dimer has been investigated experimentally in the microwave (MW)(2) and infrared (IR) (3,4) (via the ν_3 CH asymmetric stretching vibration of acetylene) ranges and theoretically by *ab initio* methods (5,6). Very recently, a combination band was reported and analysed by Moazzen-Ahmadi and coworkers when investigating the region of the CO_2, ν_3 fundamental band ($\sim 2349\text{ cm}^{-1}$) of this $C_2H_2-CO_2$ dimer (7). This *c*-type band was assigned as a resulting from the excitation of the torsional mode between the two monomers. The torsional motion is also represented on Figure 1.

The story about the isoelectronic $C_2H_2-N_2O$ complex is similar, except for the absence of *ab initio* investigation. MW (8-10) and IR (11) studies were published demonstrating planar C_s structure with the two linear monomers almost parallel. A combination, torsional band was also identified by Moazzen-Ahmadi and coworkers, in the region of the N_2O, ν_1 fundamental band (12). For both $C_2H_2-CO_2$ and $C_2H_2-N_2O$ dimers the combination band is weaker than the corresponding fundamental band, about 20 times in the case

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4 of $C_2H_2-CO_2$. In these studies, the torsional frequency, $\tilde{\nu}_{torsion}$, was determined
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7 to be around 44 cm^{-1} for both species, actually corresponding to the separation
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9 between the origin of the bands with and without torsional excitation,
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12 $\Delta\tilde{\nu}_0^{torsion}$.
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15 Both dimers were also investigated at ULB, now in the near IR region
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17 around $1.5\ \mu\text{m}$. The 2CH overtone band was observed in each case, showing
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19 well resolved but perturbed rotational structure. More lines could be assigned
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21 in $C_2H_2-CO_2$ (13) than in $C_2H_2-N_2O$ (14). We did not search for additional bands
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23 in the range at the time, since they were expected to be even weaker than the
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25 overtone bands. We recently significantly improved on the performances of the
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27 instrumental set-up used to record the $1.5\ \mu\text{m}$ spectral range of dimers (15)
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29 and decided to perform new experiments. The goal was to observe combination
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31 bands similar to those reported in the lower IR region. We report on these
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33 successful experiments in the present contribution. The experimental results
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35 and analysis are presented in section 2 and discussed in section 3 which also
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37 concludes the present report.
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52 **2. Results and analysis**

53 **2.1. Experiments**

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57 The spectra were recorded using the CW-cavity ring down spectroscopy
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(CW-CRDS) facilities in the FANTASIO+ set-up (for “Fourier trANsform, Tunable diode and quadrupole mAss spectrometers interfaced to a Supersonic expansIOn”). The latest version of FANTASIO+ is described in (15,16) and the detailed instrumental features are not repeated here. Different from the previous experiments on C_2H_2 - CO_2 and C_2H_2 - N_2O was first the use of two large turbomolecular pumps (Leybold MAG W3200 CT, teflon coated) to produce the expansion, rather than one. New super-mirrors also allowed the ring down time to be increased from about 20 to 130 μs . The number of passes is now around 72000, corresponding to ~ 720 m effective absorption path in the cooled gas, below the ~ 1 cm long slit. A more accurate calibration procedure, of the order of ± 0.0005 cm^{-1} , is also used to measure line positions. Optimal conditions for C_2H_2 - CO_2 were found to be: $P_{in} = 0.018$ hPa (residual), $P_{out} = 639$ hPa (reservoir), and injection flows, in sccm, of 222 for CO_2 , 62 for C_2H_2 , and 4604 for Ar. For C_2H_2 - N_2O , they were: $P_{in} = 1.7$ hPa (residual), $P_{out} = 633$ hPa (reservoir), and injection flows, in sccm, 210 for N_2O , 62 for C_2H_2 , and 4604 for Ar. All gases are from high purity commercial bottles. The range 6580 to 6596 cm^{-1} was recorded in both cases and a portion of the spectra is presented in Figures 2 and 3, demonstrating the presence of combination bands. In both cases, acetylene monomer lines were also observed, usually corresponding to the strongest lines in Figures 2 and 3 (17,18). We checked that C_2H_2 -Ar (19) is not observed in the range investigated.

2.2 Analysis

The two newly reported combination bands are *c*-type bands. We attempted their rotational analysis using Colin Western's PGOPHER software (20). Since assignment and fitting problems were previously encountered in the main, 2CH bands, we did not expect being able to perform a full analysis of the combination band using a rigid asymmetric top rotor Hamiltonian. Indeed, many perturbations were encountered which severely limited the assignment procedure. We therefore focused on low *J*, *K* lines, aiming at determining the band origin, in particular. The assigned data are listed in Tables 1 and 2 for C₂H₂-CO₂ and C₂H₂-N₂O, respectively. They were fitted constraining ground state (GS) constants to their literature values (7)(14). Resulting upper state constants are listed in Table 3 for both species. The rms deviation of the fit was 1.8×10^{-3} and 1.5×10^{-3} cm⁻¹ for C₂H₂-CO₂ and C₂H₂-N₂O, respectively. The comparison between observed and simulated spectra is presented in Figures 2 and 3. The simulations were visually found to agree best with the observed spectra for $T_{\text{rot}} = 18$ K, determined by trial and error. The 1:3 intensity alternation for even : odd lower *K_a* values is included in the simulation for C₂H₂-CO₂.

3. Discussion

The separation ($\Delta\tilde{\nu}_0$) between the 2CH band origin provided in the literature (13)(14) and the present combination band origin is listed in Table 3, for each dimer. Both values are very similar ($\sim 40 \text{ cm}^{-1}$). They are furthermore very close to $\Delta\tilde{\nu}_0^{\text{torsion}}$ obtained in the same way using the lower energy bands in the literature ($\sim 44 \text{ cm}^{-1}$). Since the two bands presently analyzed are also of *c*-type and thus involve out-of-plane excitation as well, there is no doubt that the same torsional vibrational mode is involved in all cases. All values $\Delta\tilde{\nu}_0^{\text{torsion}}$ are gathered in Table 4.

Using a conventional expression for vibrational energy in function of vibrational frequencies ($\tilde{\nu}_i$) and anharmonicities (x_{ij})

$$G(v_i) = \sum_i \tilde{\nu}_i v_i - \sum_{i \leq j} x_{ij} v_i v_j \quad (1)$$

then one readily finds that

$$x_{CH/torsion} = \frac{1}{2} x_{CO/torsion} + 2 \text{ cm}^{-1} \quad (2)$$

The present results also nicely confirm that carbon dioxide and nitrous oxide behave very similarly upon complexation with acetylene. **They further**

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4 show that the nature of the intermolecular bonding seems not to be
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6 significantly affected by vibrational excitation, at least for those stretching
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8 excitation study cases investigated in the literature and in the present work.
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15 The observation of the 2CH + torsion combination band is an amazing
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17 result. It is indeed a very weak band in the near infrared spectral range
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19 corresponding to triple vibrational excitation in a weakly bound dimer. The
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21 torsional mode could have been expected to favor dissociation, considering
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23 that the upper state energy is already about 20 times the dissociation energy.
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25 Nevertheless, a rotationally resolved, *c*-type band was observed for each dimer
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27 that could be analyzed for low *J*- and *K*-lines, producing upper state constants
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29 and band origins. We checked that the sub-Doppler line widths of the lines in
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31 the 2CH + torsion combination band are very similar to those of the main
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33 2CH band, indicating very similar life times. The dimer with 2CH excitation is
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35 thus not significantly affected by the additional torsional excitation.
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47 The present experimental result confirms the ultra-high sensitivity of the
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49 set-up. Indeed the previously reported combination bands, all weak, were close
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51 to much stronger fundamental bands and furthermore observed using pulsed,
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53 more efficient supersonic expansions. One should also notice that similar
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55 combination bands were not reported in the literature in association to 1CH
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4 excitation in the acetylene unit, further confirming the quality of the present
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7 experimental results.
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12 So, in conclusion, the present investigation was driven by recent literature
13 reporting on the observation of torsional combination bands in $C_2H_2-CO_2$ and
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15 $C_2H_2-N_2O$ close to fundamental bands. We have observed similar bands in
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17 association to 2CH excitation, in the near-infrared spectral range. Triple
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19 vibrational excitation in van der Waals complexes is thus possible and can be
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21 investigated, way above the dissociation energy. Rotational constants were
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23 obtained. The torsional frequency is about 40 cm^{-1} in both $C_2H_2-CO_2$ and
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25 $C_2H_2-N_2O$. It is hoped that the present results will stimulate theoretical
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27 investigations aiming at producing reliable potential energy surfaces in these
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29 excited regions to help in further investigations, including more complete
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31 rotational analyses of the bands.
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48
49 It is our great pleasure to dedicate this paper to Prof. Gianfranco Di
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Figure Captions

Figure 1: On scale structure of the $C_2H_2-CO_2$ van der Waals hetero dimer. The arrows (not on scale) indicate the torsional vibration assuming two rigid monomer entities.

Figure 2: Central portion of the $2CH +$ torsion combination band in $C_2H_2-CO_2$, observed (top) and simulated at 18 K rotational temperature (bottom). Stronger lines are from the acetylene monomer. The experimental conditions are detailed in the text.

Figure 3: Central portion of the $2CH +$ torsion combination band in $C_2H_2-N_2O$, observed (top) and simulated at 18 K rotational temperature (bottom). Stronger lines are from the acetylene monomer. The experimental conditions are detailed in the text.

Table legends

Table 1: Assigned and fitted lines in the 2CH + torsion combination band in C₂H₂-CO₂. Wavenumbers are in cm⁻¹.

Table 2: Assigned and fitted lines in the 2CH + torsion combination band in C₂H₂-N₂O. Wavenumbers are in cm⁻¹.

Table 3: Upper and GS state constants (in cm⁻¹) in the 2CH + torsion combination band in C₂H₂-CO₂ and C₂H₂-N₂O. Uncertainties in parentheses are 1σ from the least-squares fits in units of the last quoted digit. Δν̃ is the separation with the 2CH band origin.

Table 4: Separation (Δν̃₀^{torsion} in cm⁻¹) between origins of bands with and without torsion excitation in C₂H₂-CO₂ and C₂H₂-N₂O.

Table 1

Wavenumber	J'	Ka'	Kc'	J''	Ka''	Kc''
6589.8900	4	1	4	4	0	4
6589.7540	9	1	9	9	0	9
6589.7420	10	1	10	10	0	10
6589.7310	11	1	11	11	0	11
6589.6748	17	1	17	17	0	17
6589.6470	20	1	20	20	0	20
6589.1949	1	0	1	2	1	1
6589.5930	2	0	2	2	1	2
6589.6140	3	0	3	3	1	3
6589.6370	4	0	4	4	1	4
6589.6658	5	0	5	5	1	5
6589.6830	16	0	16	16	1	16
6589.6748	17	0	17	17	1	17
6589.6658	18	0	18	18	1	18
6589.6564	19	0	19	19	1	19
6589.6470	20	0	20	20	1	20
6590.3960	2	2	1	2	1	1
6590.2960	4	2	3	4	1	3
6590.2288	5	2	4	5	1	4
6590.1514	6	2	5	6	1	5
6590.0672	7	2	6	7	1	6
6589.9810	8	2	7	8	1	7
6589.8972	9	2	8	9	1	8
6589.8230	10	2	9	10	1	9
6589.7560	11	2	10	11	1	10
6589.6564	13	2	12	13	1	12
6589.6172	14	2	13	14	1	13

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6589.5861	15	2	14	15	1	14
6589.5595	16	2	15	16	1	15

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Table 2

Wavenumber	J'	Ka'	Kc'	J''	Ka''	Kc''
6590.0944	5	1	4	6	0	6
6590.6275	10	1	10	10	0	10
6590.6483	9	1	9	9	0	9
6590.6733	8	1	8	8	0	8
6590.7015	7	1	7	7	0	7
6590.7352	6	1	6	6	0	6
6590.7687	5	1	5	5	0	5
6590.8111	4	1	4	4	0	4
6590.8518	3	1	3	3	0	3
6590.8874	2	1	2	2	0	2
6590.2822	0	0	0	1	1	0
6590.4835	2	0	2	2	1	2
6590.4996	3	0	3	3	1	3
6590.5405	5	0	5	5	1	5
6590.5581	6	0	6	6	1	6

Table 3

	$\text{C}_2\text{H}_2\text{-CO}_2$		$\text{C}_2\text{H}_2\text{-N}_2\text{O}$	
	GS ^{*a}	2CH+torsion	GS ^{*b}	2CH+torsion
$\tilde{\nu}_0$		6589.78290(74)		6590.69147(94)
A	0.295813	0.29990(33)	0.313359399	0.3141(12)
B	0.09543775	0.092380(30)	0.09446473	0.090569(95)
C	0.07193428	0.0718100(34)	0.07231532	0.072179(25)
$10^6 \times \Delta_K$	-5.66	-5.66*	0.825	0.825*
$10^6 \times \Delta_{JK}$	2.08	2.08*	1.603	1.603*
$10^7 \times \Delta_J$	2.68	2.68*	4.585	4.585*
$10^6 \times \delta_K$	-4.86	-4.86*	2.036	2.036*
$10^8 \times \delta_J$	1.01	1.01*	11.226	11.226*
$10^3 \times \text{rms}$		1.8		1.5
$\Delta\tilde{\nu}_0$		40.491(2)		40.778(2)

* Constrained in the fit.

^a Lauzin *et al.* (7)

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4 ^b Didriche *et al.* (14)
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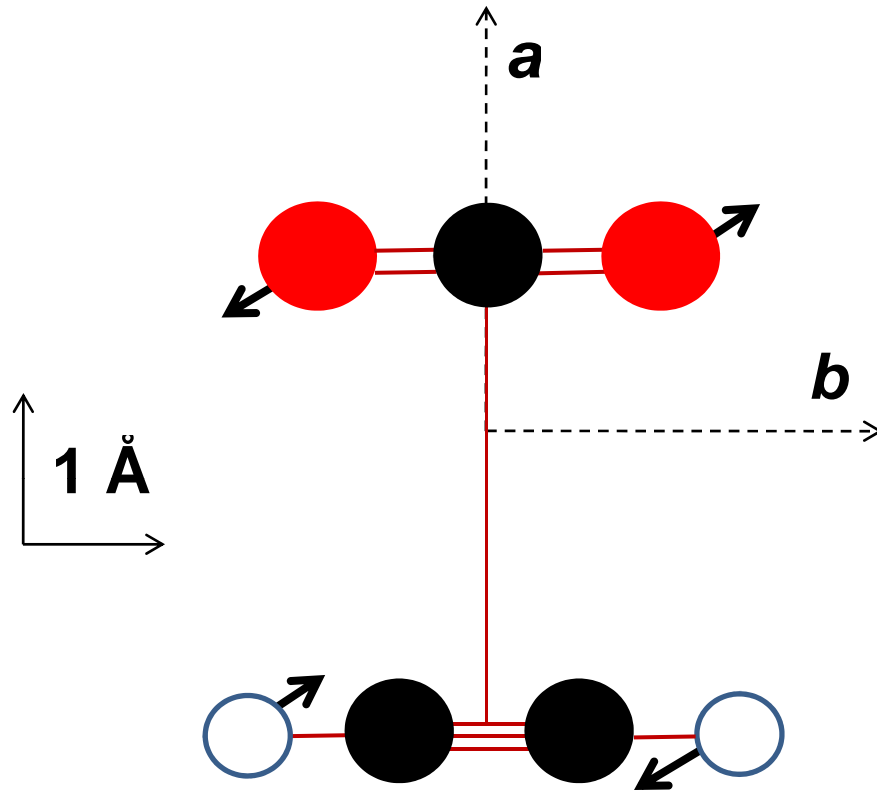
Table 4

	$\Delta\tilde{\nu}_0^{torsion}$
CO ₂ - C ₂ H ₂ (ν_3 , CO ₂)	44.385 ^a
N ₂ O - C ₂ H ₂ (ν_1 , N ₂ O)	44.372 ^b
CO ₂ - C ₂ H ₂ (2CH, C ₂ H ₂)	40.491 ^c
N ₂ O - C ₂ H ₂ (2CH, C ₂ H ₂)	40.778 ^c

^a Lauzin *et al.* (7)

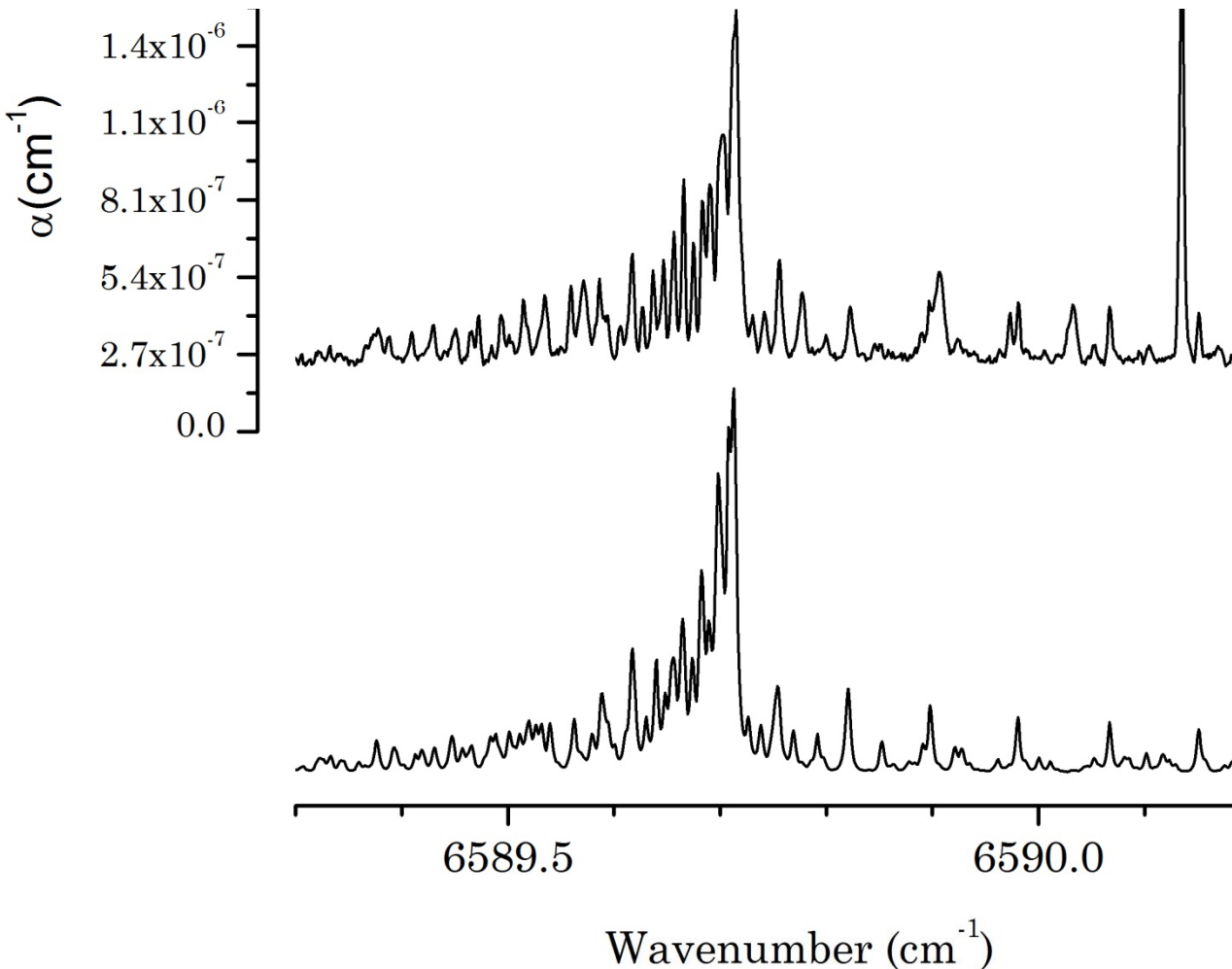
^b Dehghany *et al.* (12)

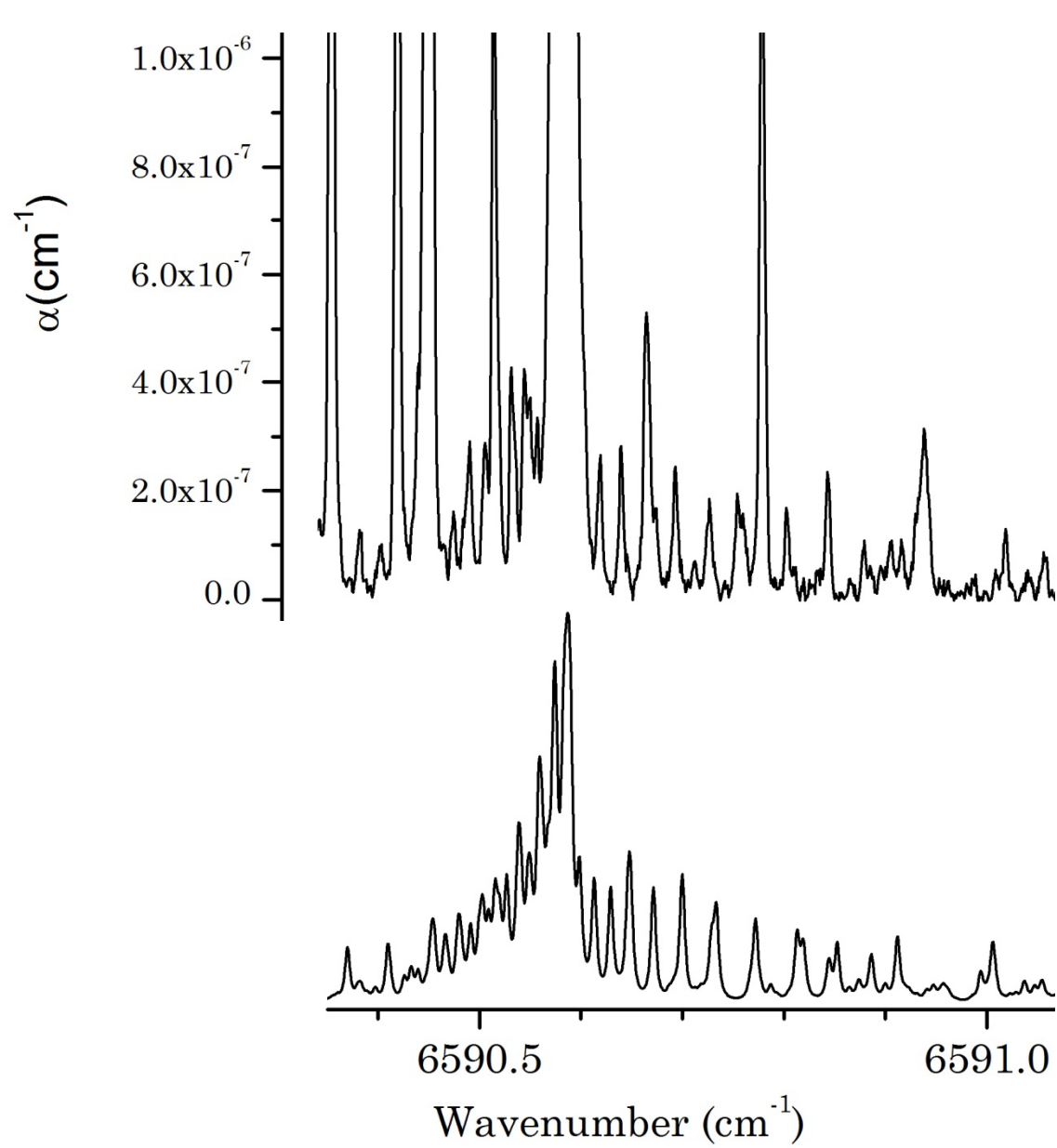
^c This work



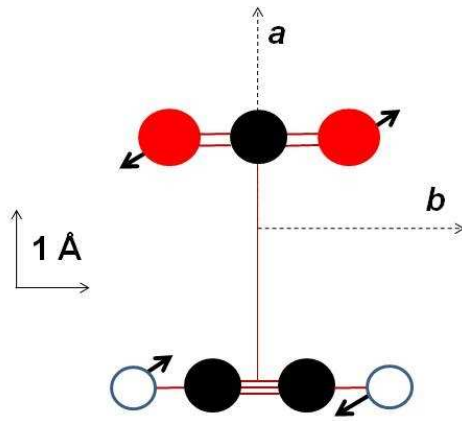
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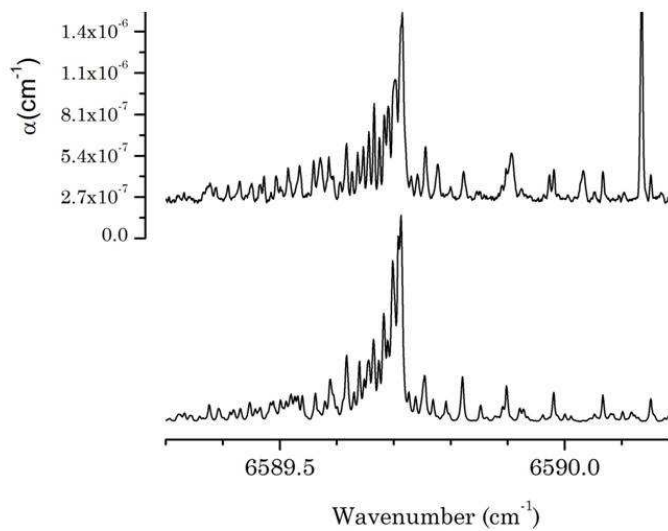


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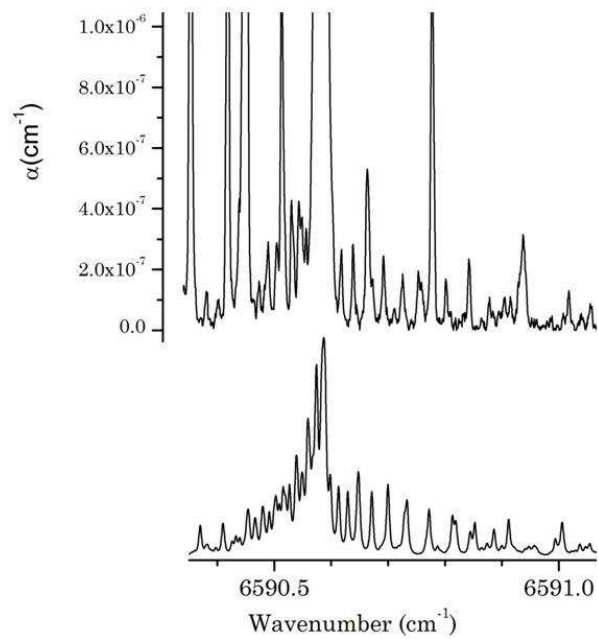
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